IUCLID 5
Guidance and Support

Installation Guide for IUCLID 5 Version 5.3
Stand-alone Application

Custom Installation on Microsoft® Windows®

August 2011

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Chapter 1. Introduction

IUCLID 5 can be installed either as a stand-alone application, or in a multi-user environment that uses client-server architecture. The purpose of this document is to describe how to install manually, a single stand-alone application version of the IUCLID 5.2 software onto a computer running Microsoft® Windows® (hereafter referred to as Windows). The installation is performed by ensuring that prerequisite software is installed, copying files to the computer and, if necessary, making some configuration changes that are explained in this document. If the instructions in this document are followed exactly, no prior specialist knowledge is required of either the IUCLID 5 software, or the software components required to run it.

The stand-alone installation of IUCLID 5 should be carried out manually if you want to use a database and version of Java other than those that are used with the IUCLID 5 installer for Windows. For example, the database Oracle rather than PostgreSQL.

If you encounter any problems during the installation that cannot be solved using information in this manual, or the documentation of third party softwares; before contacting ECHA Helpdesk, please try the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.

1.1. Hardware requirements

The following requirements are provided as only a guide.

- At least 1 GB of mother board RAM (2 GB for Windows Vista®)
- Pentium Core 2 duo or equivalent

An installation of IUCLID 5 will most likely run on a lower specified machine but the performance might not be satisfactory. The requirements depend in part on the version of Windows and the IUCLID plugins that are in use. For example, using the Query Tool plugin will increase the resources required to obtain a reasonable running speed; especially on a large database.

1.2. Software requirements

The software prerequisites for the installation are as follows:

- Windows preferably with knowledge of the administrator password.

  It is recommended to carry out the installation from a standard type of Windows user account, rather than an administrator. You will be prompted to enter the administrator password where necessary.

- Java - J2SE Runtime Environment v6
- Database - PostgreSQL 8.2, 8.3, 8.4 (recommended) or 9; or Oracle 10g. IUCLID 5 works with either. You do not need both PostgreSQL **and** Oracle.

  The Oracle driver for Java is no longer supplied with the IUCLID installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the oracle web site and installed in the appropriate folder. For example, for Java 1.6 and Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`. For use with Tomcat, the driver must be placed in Tomcat's library folder, e.g. `Tomcat\lib`.

- The IUCLID 5 manual workstation installation package, version 5.3, can be downloaded without charge from the IUCLID 5 web site.
- Once you have completed the installation of IUCLID 5, you should test it by starting and configuring it. The configuration requires access to at least a legal entity file (LEOX). The creation of a LEOX is described on the IUCLID 5 web site where the installation software is published. In addition, it is recommended to upload a set of reference substances and the EC inventory. These are also available from the web site at which the IUCLID 5 software is published.

Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set*, a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

For more information regarding system requirements, see the FAQ on the IUCLID web site located at http://iuclid.eu.

Chapter 2. Making a fresh installation of IUCLID 5

If Java and PostgreSQL are already installed, go straight to section Section 2.1.3, “Configuration of PostgreSQL”.

2.1. Installation of Software Required by IUCLID 5

The installation of third party software is described by the respective publishers. Please refer to their web sites for full instructions.

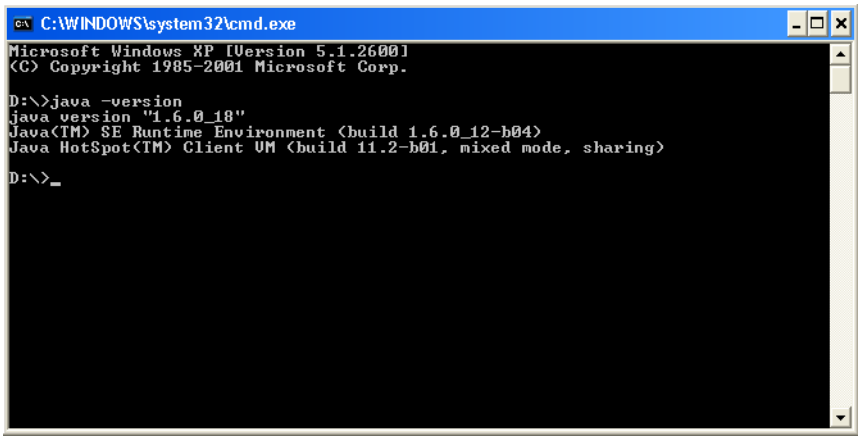
2.1.1. Installation of Java

1. Verify whether Java (JRE) of the correct version is installed on the computer to which IUCLID will be installed:

   Open a command prompt (Start # Run… # Open: cmd). At the command prompt, enter the following:

   ```
   java -version
   ```

   Figure 2.1. Check version of Java

   
   C:\WINDOWS\system32\cmd.exe
Microsoft Windows XP [Version 5.1.2600]
(C) Copyright 1985-2001 Microsoft Corp.
D:\>java -version
java version "1.6.0_18"
Java(TM) SE Runtime Environment (build 1.6.0_12-b04)
Java HotSpot(TM) Client VM (build 11.2-b01, mixed mode, sharing)
D:\>

2. If a message similar to the one shown in the screen shot above is not shown, or the version of Java is not 1.6 or higher, install the latest version. It can be downloaded from the Sun site at www.java.com.

Figure 2.2. Installation wizard for Java

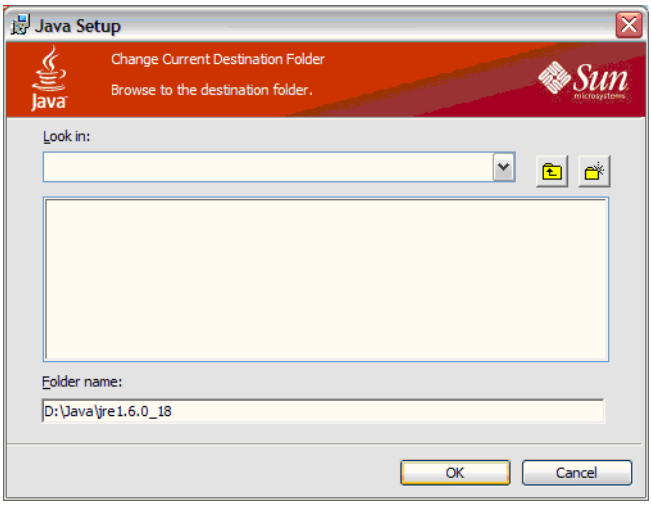


Figure 2.3. Choose installation directory for Java

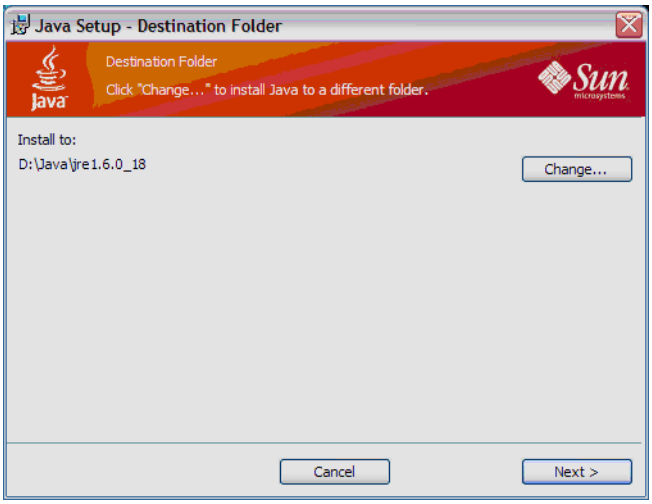
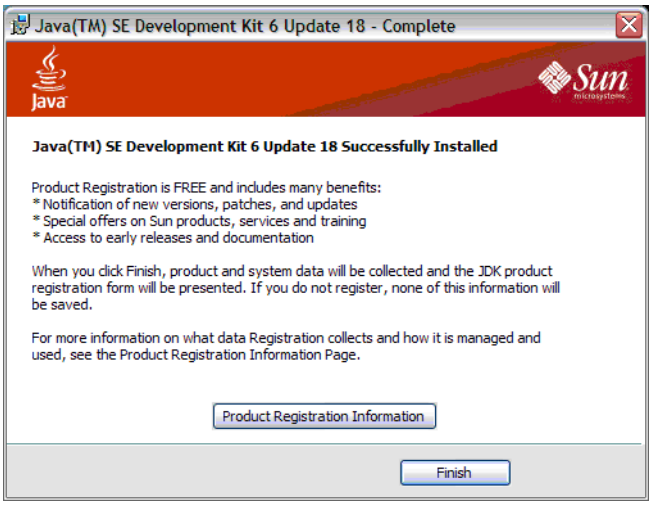


Figure 2.4. Installation of Java is complete


Java(TM) SE Development Kit 6 Update 18 - Complete
Java
Sun
Java(TM) SE Development Kit 6 Update 18 Successfully Installed
Product Registration is FREE and includes many benefits:
* Notification of new versions, patches, and updates
* Special offers on Sun products, services and training
* Access to early releases and documentation
When you click Finish, product and system data will be collected and the JDK product registration form will be presented. If you do not register, none of this information will be saved.
For more information on what data Registration collects and how it is managed and used, see the Product Registration Information Page.
Product Registration Information
Finish

2.1.2. Installation of PostgreSQL

If either version 8.2, 8.3 or 8.4 of PostgreSQL is already installed and running as a service with a user `postgres`, the existing installation can be used. There is no need to upgrade to 9, although 9 is supported. If PostgreSQL is not already installed on the computer, or you would like to upgrade to 9, download PostgreSQL 9 from the site www.postgresql.org/download and install it. The web site of PostgreSQL offers a range of alternative ways to download and install the PostgreSQL software. The screen shots shown below show the use of the *one click installer* available from the PostgreSQL web site. An example of the file name of the installer is *postgresql-9.0.4-1-windows.exe*.

The default fresh installation of PostgreSQL, made using the *one click installer*, automatically starts PostgreSQL as a service, creates the user `postgres` if necessary, and supplies administration tools (e.g. pgAdmin III) that can be used to create the database. If the installer creates the superuser `postgres`, you will have to create a password for it, as shown in the figure below, and enter it later into the configuration file for IUCLID 5.

Figure 2.5. Installer for PostgreSQL

Figure 2.6. Installation directory for PostgreSQL

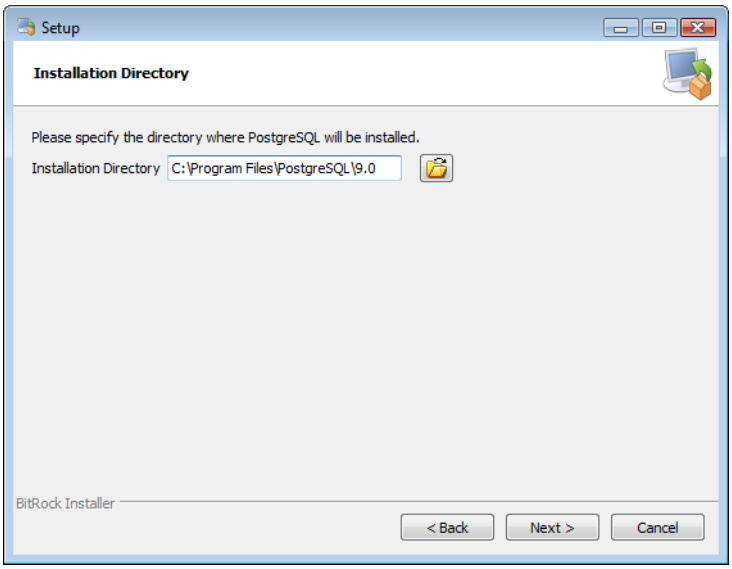


Figure 2.7. Data directory for PostgreSQL

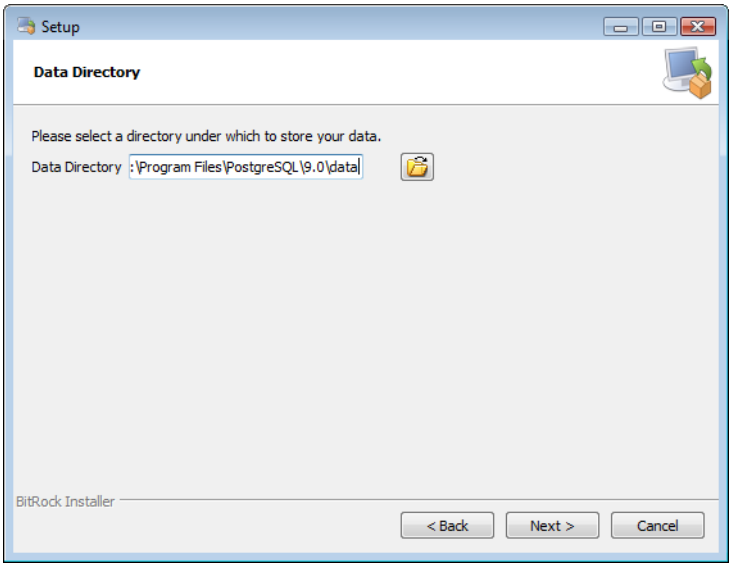


Figure 2.8. Password for the database superuser (postgres) and the Windows service account (postgres)

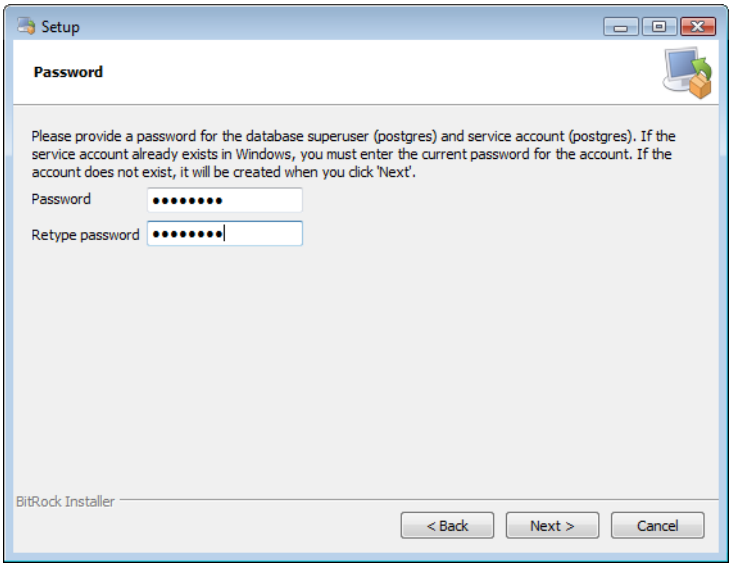

Setup
Password
Please provide a password for the database superuser (postgres) and service account (postgres). If the service account already exists in Windows, you must enter the current password for the account. If the account does not exist, it will be created when you click 'Next'.
Password
Retype password
BitRock Installer
< Back
Next >
Cancel

Figure 2.9. Port number for PostgreSQL

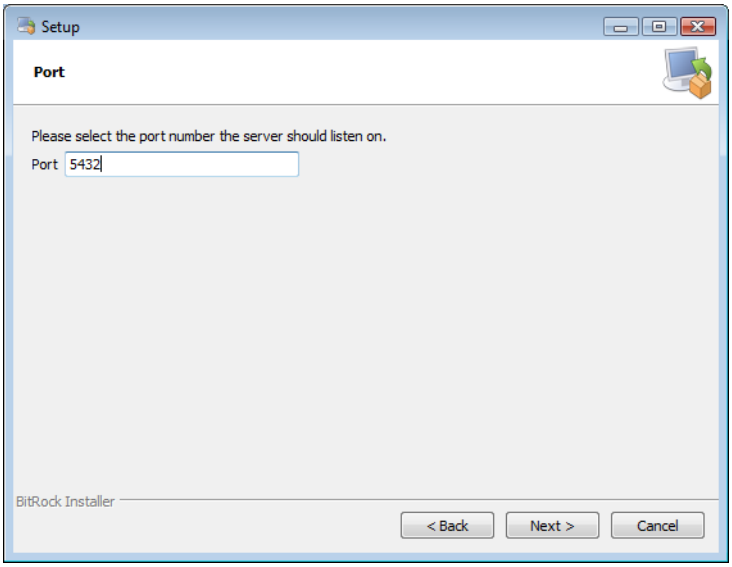


Figure 2.10. Set the default locale for PostgreSQL

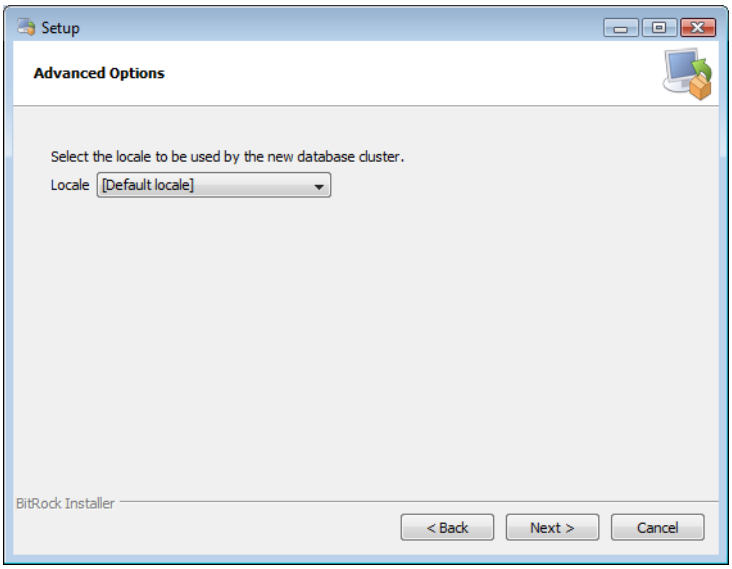


Figure 2.11. Confirm installation of PostgreSQL

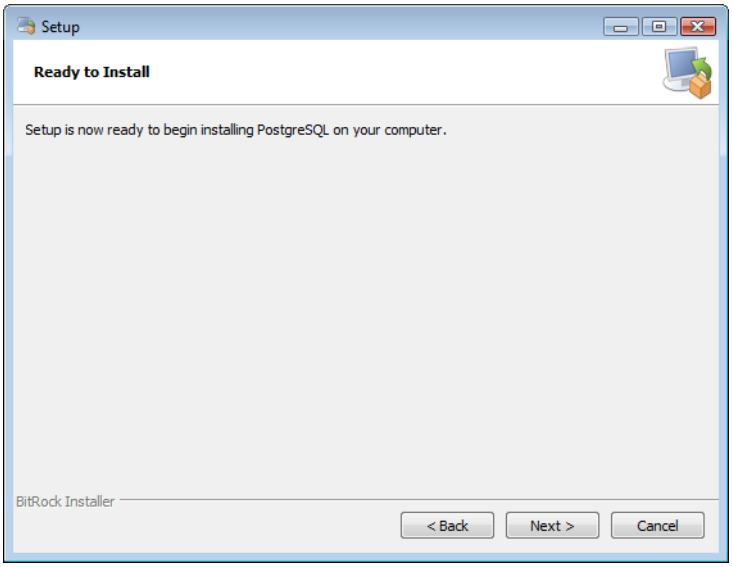


Figure 2.12. Installation of PostgreSQL in progress

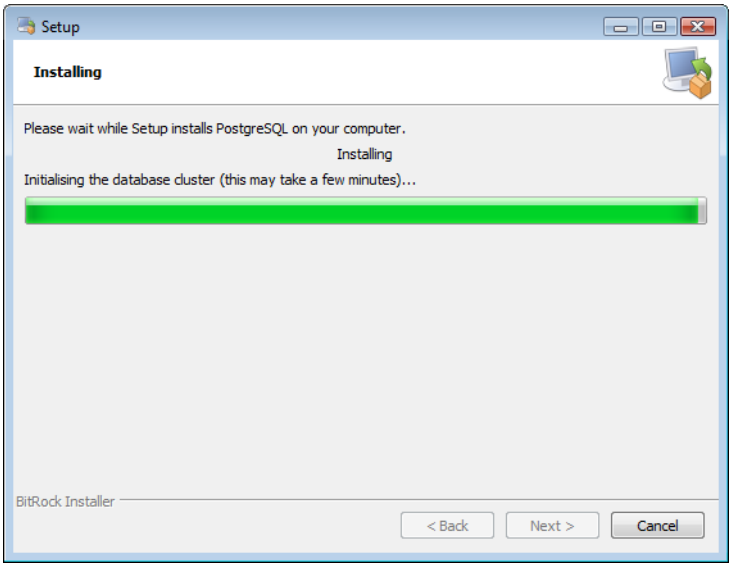


Figure 2.13. Installation of PostgreSQL complete

Setup
PostgreSQL
Packaged by:
EnterpriseDB
The Enterprise PostgreSQL Company
Completing the PostgreSQL Setup Wizard
Setup has finished installing PostgreSQL on your computer.
Launch Stack Builder at exit?
Stack Builder may be used to download and install additional tools, drivers and applications to complement your PostgreSQL installation.
< Back
Finish
Cancel

2.1.3. Configuration of PostgreSQL

A new user and a new database need to be created.

Tip

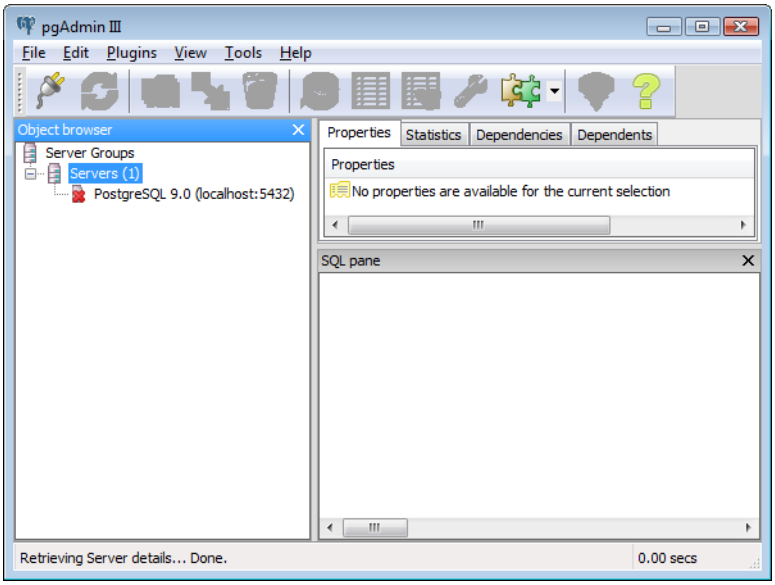
IUCLID 5 is configured by default to connect to the database using username:*iuclid5* and password:*iuclid5*. It is convenient to specify the same password now, and change it later when the application is set up correctly.

Important

Take note of the password of this user. This user name and password will be needed later to connect IUCLID 5 to the database.

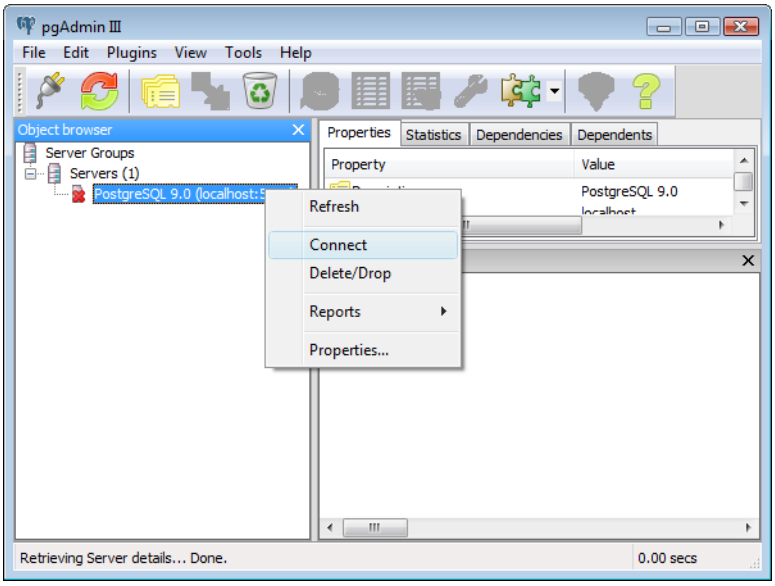
The program pgAdmin III can be used to create the database as follows. Start pgAdmin III from the menu *Start / All Programs / PostgreSQL9.0*. After the splash screen has appeared and you have closed the pop-up window that shows usage tips, the following screen is shown.

Figure 2.14. pgAdmin III interface on first opening



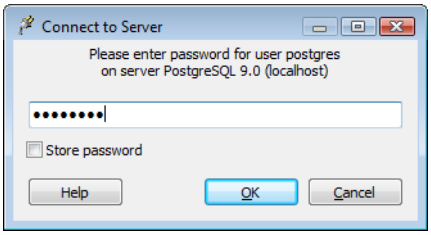
Right-click the text *PostgreSQL 9.0 (localhost:5432)* that is under the word *Servers* highlighted in blue in the figure above. Select *connect* as shown below.

Figure 2.15. Connect pgAdmin III to PostgreSQL as user postgres



Enter the password for user *postgres* as given in the postgres installer Figure 2.8, “Password for the database superuser (postgres) and the Windows service account (postgres)” then click *OK*. It is recommended to store the password to facilitate future access.

Figure 2.16. Authenticate the user postgres



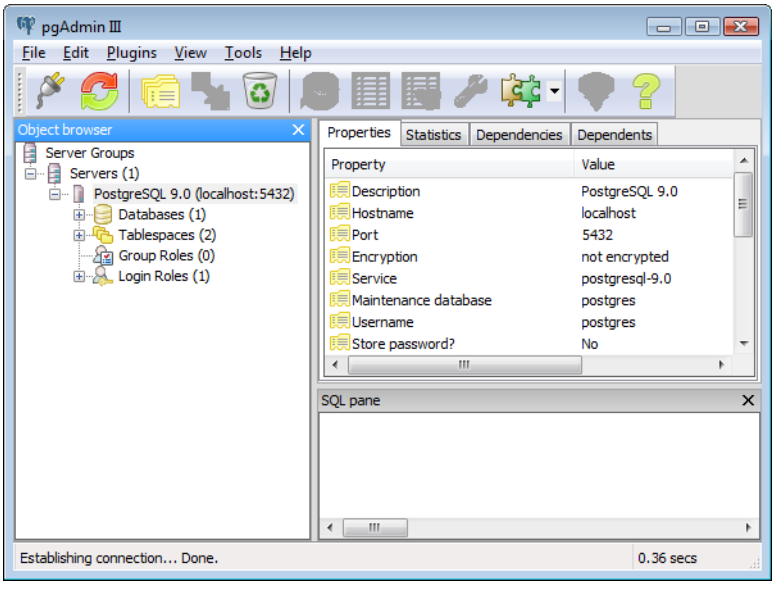
If you elect to save the password, the following warning might be displayed. Click *OK*

Figure 2.17. Saving passwords Warning

Guru Hint - Saving passwords
Saving passwords
WARNING: You have opted to save your password. It will be stored in plain text in your home directory on *nix systems, or in your user profile on Windows. If you do not want this to happen, please press the Cancel button.
pgAdmin uses PostgreSQL's 'pgpass' mechanism to store your passwords. On *nix systems, the password will be stored in ~/.pgpass, whilst on Windows systems it will be stored in %APPDATA%\PostgreSQL\pgpass.conf (%APPDATA% is the 'Application Data' folder in your user profile). This mechanism is used by default by all programs that use the libpq library to access the server, which includes command line applications such as pg_dump and pg_restore, other GUI applications, and drivers such as psqlODBC. This means that those applications may automatically connect to the server using your stored password. If you do not want this to happen, you should not use the Store Password option in pgAdmin.
Do not show this hint again
Help
OK
Cancel

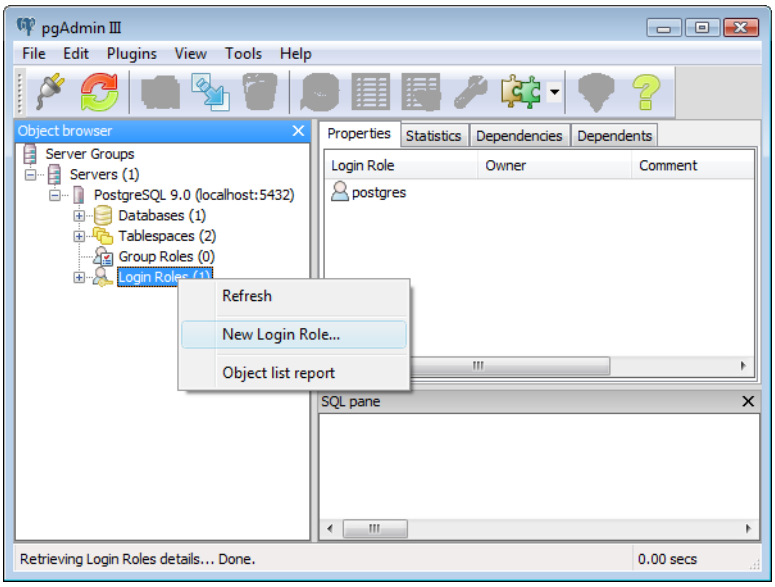
Expand the tree for *PostgreSQL 9.0 (localhost:5432)* by clicking the plus sign that has just appeared next to it, as shown in the figure below.

Figure 2.18. Initial screen in pgAdmin III



Right-click on *Login Roles* and select *New Login Role...*.

Figure 2.19. Select create a new user option

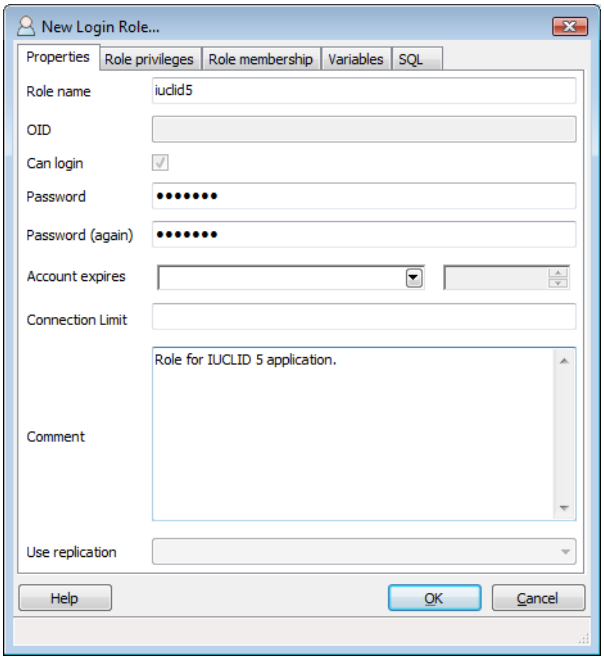


Enter the role name *iuclid5*. Set the password.

Important

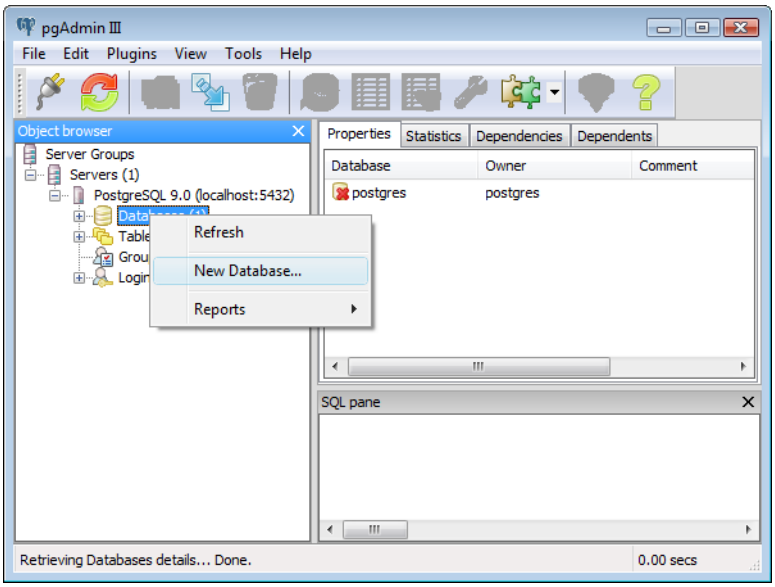
Make a note of the user name and password. They are referred to later in the installation, in section Section 2.2, “Installation of IUCLID 5” [15]. We recommend using `iuclid5` as both the user name and the password.

Figure 2.20. Create a new role (i.e. a user) with the name iuclid5



Request a new database by right-clicking the text *Databases* and selecting *New Database...* as shown in the figure below.

Figure 2.21. Request a new database in pgAdmin III

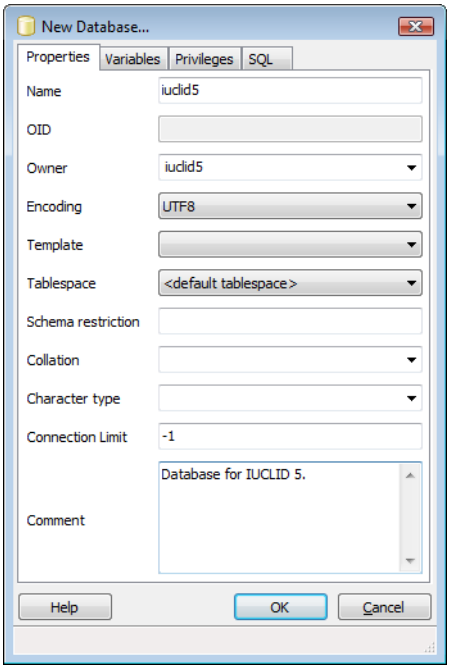


Enter the details you require. Normally these are only name=iuclid5 and owner=iuclid5. The encoding should be UTF8. Click *OK*.

Important

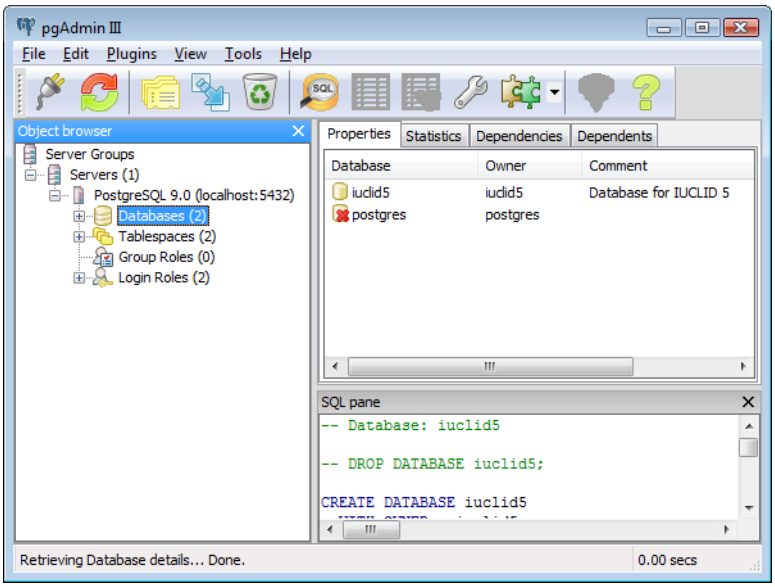
Make a note of the database name. It is referred to later in the installation, in section Section 2.2, “Installation of IUCLID 5” [15]. We recommend using the name `iuclid5`.

Figure 2.22. Enter the details of IUCLID 5's database into pgAdmin III



As you can see from the figure below, there is now a new database named *iuclid5*.

Figure 2.23. List of databases in pgAdmin III



You can now close *pgAdmin III* and move directly to the installation of IUCLID 5.

2.1.4. Installation and Configuration of Oracle

The installation and configuration of an Oracle database are out of the scope of this document. The parameters that must be defined for IUCLID 5 are shown below, in an extract from the settings file for IUCLID 5. This file, named *workstation.properties*, can be found in the installation directory of IUCLID 5 as described later in this document:

Settings for using ORACLE 10g

hibernate.connection.username=<username>

hibernate.connection.password=<password>

hibernate.connection.driver_class=oracle.jdbc.driver.OracleDriver

hibernate.connection.url=jdbc:oracle:thin:@localhost:1521:iuclid5

hibernate.hbm2ddl.auto=validate

hibernate.dialect=eu.eca.iuclid.server.system.persistence.ExtendedOracle9Dialect

hibernate.jdbc.use_streams_for_binary=false

2.2. Installation of IUCLID 5

Unzip the archive that contains the software for the manual installation of IUCLID 5. Do not unzip or change the relative location of any of the plugin archives. Create an installation directory for IUCLID 5 somewhere convenient (for example `C:\ Program Files \ IUCLID5`). Copy the directory `workstation` and all its contents into the installation directory. Use your favourite text editor to edit the file `workstation.properties` so that it conforms to your system. If you experience difficulties in saving changes to the properties file, try explicitly granting write access for it to standard local users. This can be done by right-clicking the file, selecting *properties / security*, highlighting your user group or user name, then ticking the box *allow* for *write*. You will need to supply an administrator password. The *write* permission can be revoked after your IUCLID 5 has been successfully configured.

If you are using PostgreSQL with only default values, the changes required for the properties file can be as simple as adding the password for the user *postgres*, as follows:

hibernate.connection.password=<password for the user that connects to the database, e.g. postgres>

For the parameters that relate to a type of database that is not being used, place a # symbol at the start of each line. The default configuration file delivered with the installation is shown below:

$Id: workstation.properties,v 1.5 2007/05/10 09:10:04 hallerp Exp $

Default workstation properties over-riding hard coded defaults in application

application.type=workstation scavenger.frequency=60 session.timeout=7600

Settings for using PostgreSQL#

hibernate.connection.username=iuclid5

hibernate.connection.password=iuclid5password

hibernate.connection.driver_class=org.postgresql.Driver

hibernate.connection.url=jdbc:postgresql://localhost:5433/iuclid5

hibernate.hbm2ddl.auto=validate

hibernate.dialect=org.hibernate.dialect.PostgreSQLDialect

hibernate.jdbc.use_streams_for_binary=false

Settings for using ORACLE 10g

#hibernate.connection.username=iuclid5a

#hibernate.connection.password={aXVjbGlkNWE=}

#hibernate.connection.driver_class=oracle.jdbc.driver.OracleDriver

#hibernate.connection.url=jdbc:oracle:thin:@localhost:1521:iuclid5

#hibernate.hbm2ddl.auto=validate

#hibernate.dialect=eu.eca.iuclid.server.system.persistence.ExtendedOracle9Dialect

#hibernate.jdbc.use_streams_for_binary=false

2.3. Installation Check List - Example

What follows is a check list of an example of the sequence of actions required to make a fresh installation of IUCLID 5, Java and the PostgreSQL database. It contains all that an experienced Windows administrator needs to know to perform such an installation. More detailed instructions are given later in this document. To use an Oracle database, the procedure is similar.

1. Install the latest JRE for your version of Windows from Sun, available without charge within the limits of the license, from the site www.java.com.

2. Install the latest PostgreSQL for your version of Windows, available without charge within the limits of the license, from www.postgresql.org/download. If a user *postgres* does not exist already, the wizard will create one and ask you to give it a password. Remember the password for subsequent steps.

3. Create a database named *iuclid5*. A convenient way to do this is using the graphical admin tool pgAdmin III that comes with PostgreSQL.

4. Create an installation directory for IUCLID 5 somewhere convenient, for example C:\Program Files\IUCLID5.

5. Copy into the installation directory, all the contents of the directory named `workstation` supplied in the zipped archive of the IUCLID 5 download. Do not unzip any of the plugin files.

6. Edit the supplied IUCLID 5 settings file, `workstation.properties` so that it contains the password for the Windows user that connects to the database, e.g.:

   hibernate.connection.username=postgres

   hibernate.connection.password=<password>

7. Start IUCLID 5 by running the executable file `iuclid5.cmd` from the installation directory. If IUCLID 5 does not run first time, check that PostgreSQL is running as a service and that there is a user named *postgres*.

8. Follow the instructions to configure IUCLID 5. If you need detailed help, see the help pages that can be accessed from the link denoted by a question mark, *?* at the bottom left of the page of the configuration wizard.

9. If the installation has been a success, create any links to `iuclid5.cmd` you might require, for example a shortcut from the Desktop. There is an icon in the installation folder that you can use with a shortcut.

Chapter 3. Upgrade

This chapter describes how to upgrade a previous version of IUCLID 5 to the most recent version of IUCLID 5.3. Dependent upon the version of IUCLID 5 that is being upgraded, there are three main scenarios in the upgrade process: upgrade from a previous version of 5.3, upgrade from any version of 5.2, and upgrade from 5.0 or 5.1. These are each described in a dedicated sub-section of this chapter. In all scenarios, before starting the upgrade, it is important to back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up functionality of the database. Making only a copy of the file system on which IUCLID is installed is not recommended as a means of backing-up.

3.1. Upgrading from a previous version of IUCLID 5.3 to the latest version of IUCLID 5.3

This section applies only to users who have an existing IUCLID 5.3 installation. If you are unsure which version you are currently using, you can read it from within the interface of IUCLID 5. Start IUCLID 5, log-in, then click 'Help' and select 'About'.

1. Save the configuration files and plug-ins from your existing IUCLID 5.3 directory to a temporary location. These are located in the following directories in your iuclid5 folder:

   `/plugins/`

   `/conf/`

2. Unzip the archive that contains the software for the manual installation of IUCLID 5. Do not unzip or change the relative location of any of the plugin archives.

3. Create an installation directory for IUCLID 5 somewhere convenient, for example `C:\Program Files\IUCLID5`.

4. Copy the directory "`workstation`" and all its contents into the installation directory.

5. Copy the plugins that were saved in step 1, over to the directory `/plugins/` in the new installation.

   Important

   When copying your pre-existing plugins, do not overwrite the new plugins that were installed with the latest version of IUCLID 5.3.

6. Replace the configuration files in the directory `/conf/` with the copies that were saved to a temporary directory in step 1.

7. Start IUCLID 5

3.2. Upgrading from IUCLID 5.2 to IUCLID 5.3

This section is relevant only if the upgrade is from IUCLID 5.2. For earlier versions, see the next section. The version can be seen from within the interface of IUCLID 5. To see the version, start IUCLID 5, log-in, then click *Help* and select *About*. The upgrade process consists of the following parts:

1. Back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up function of the database software, for example PostgreSQL.

2. Remove the executable program files for the previous version of IUCLID. Note that the plugins for IUCLID 5.2.x are not compatible with IUCLID 5.3. Therefore, they must not be copied over to the new installation.

3. Install the program files for the latest version of IUCLID 5.3 as follows. Unzip the archive that contains the software for the manual installation of IUCLID 5. Create an installation directory for IUCLID 5 somewhere convenient, for example `C:\Program Files \ IUCLID5`. Copy the directory `workstation` and all its contents into the installation directory.

4. Adapt the configuration files for IUCLID if necessary and copy to the new installation. Note that if the Oracle database is used, the file `server.properties` must contain the following entry:

```
hibernate.connection.driver_class=oracle.jdbc.OracleDriver
```

   The previous value was:

```
hibernate.connection.driver_class=oracle.jdbc.driver.OracleDriver
```

5. If the database is an Oracle database, please note that the driver for Java is no longer supplied with the IUCLID installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the Oracle web site and installed in the appropriate folder. For example, for Java 1.6 and Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`.

6. Migrate the database by running the migration tool, as described below. This is a script that is supplied along with the installation package. It migrates existing IUCLID data into the new format for IUCLID 5.3. IUCLID cannot be started until the migration tool has been run successfully.

7. Once the migration process has been completed successfully, the new version of IUCLID can be started and checked before being entered into production.

3.2.1. The migration tool

The migration tool is a script supplied with the installation package. The file name is `update.bat`. Run the script as you would any other script either from the command line, or by double-clicking on its icon in the Windows file manager. Be careful not to interrupt the running of the script, for example by closing the window associated with the script, or by shutting Windows down etc.. When the script has finished running, the window will close automatically. If the migration is interrupted, or fails, for whatever reason, the database must be restored from the back-up and the migration started again.

3.2.2. Starting IUCLID 5

If the migration tool has run successfully, you can now launch the newly installed IUCLID 5.3 by double-clicking the icon that the installer created on your Desktop, as shown below. It is also possible to launch IUCLID 5 by running the file `iuclid5.cmd` that is included in the installation directory. The initialisation process is not required. All of the data that was present in the upgraded system should be present in the new system. Therefore, it should be possible to log in to any of the user accounts from the previous system.

Figure 3.1. A shortcut to the IUCLID 5 application

3.3. Upgrading from IUCLID 5.0 / 5.1 to IUCLID 5.3

Important

There is no automatic upgrade of the database from IUCLID 5.0 / 5.1 to IUCLID 5.3. The data must be transferred manually from the old to the new database as described in the sub-section below.

Each installation of IUCLID 5 must have its own database.

3.3.1. Migration of data to IUCLID 5.3 from a previous version

Before starting to install IUCLID 5.3, all the data must be exported from the old IUCLID 5 using the Back-up plugin that is available on the IUCLID web site. The export process is essential because the exported data will later be imported into IUCLID 5.3. When it is run, the Back-up plugin asks the user to create and enter a single password. This will become the password for all the user accounts in the new installation. An exception is the account *SuperUser* which has a default password of *root*. To import the exported data into IUCLID 5.3, use the built-in Restore feature of IUCLID 5.3 that can be found from the menu File / Administrative tools. This feature allows the upload of data that was exported using the Back-up plugin on the old version of IUCLID 5.

3.3.2. Database configuration for running IUCLID 5.3 and a previous version at the same time

If you already have a previous version of IUCLID 5, it is recommended to keep it for the time being. It can be deleted in the future when you are absolutely sure that it is no longer needed. What follows is some information and advice as to how you can manage more than one version of IUCLID 5. As stated above, each installation of IUCLID 5 must have its own database. A new database must be created for IUCLID 5.3 because the structure of the database differs from that of previous versions. This requirement can be met in a variety of different ways. The following sub-sections describe two common sets of circumstances. The database for IUCLID 5.3 can be run on the same instance of the database software as a previous version of IUCLID 5, however, it must have a unique name within that instance of the database software. When IUCLID 5.3 is run for the first time on an empty database, it will automatically create all the correct tables and the initialisation wizard will start.

3.3.3. IUCLID 5.0 / 5.1 was installed using the setup-kit

The IUCLID 5 set-up kit included the database software PostgresSQL. The set-up kit installed the PostgreSQL database software, the IUCLID 5 software, and stored the database data, all under the same folder named IUCLID. The set-up kit created installations of IUCLID 5 that run PostgreSQL on a non-standard port (5433). Therefore, if an installation of IUCLID 5.3 is made with an independent installation of PostgreSQL running on the standard port (5432), it is possible to run it at the same time as an installation that was made with the set-up kit. For example, if IUCLID 5.3 is installed using the installer according to its instructions and with default settings, the new installation can be run at the same time as a previous installation that was made with the set-up kit.

3.3.4. IUCLID 5.0 / 5.1 was installed manually

In this case, you will already have an installation of PostgreSQL that is independent of IUCLID, and a database for use with IUCLID 5.0 / 5.1. There is no need to install PostgreSQL again, although you might want to take this opportunity to upgrade to PostgreSQL 9. There can be more than one database running on a single instance of the database software. Therefore, to be able to run IUCLID 5.3 and a previous version at the same time, create a new empty database for IUCLID 5.3. The name of the new database must be unique within that instance of the database software.

Chapter 4. Initialisation of an installation of IUCLID 5

This chapter describes the configuration that is required to create a working IUCLID 5 system from an installation of IUCLID 5 that has an empty database. There are two scenarios: either to create a working installation from scratch, or to load data from a back-up that was made using the built-in back-up function of IUCLID. During initialisation from scratch, reference substance data and a legal entity are uploaded into the database, and the required user accounts can be created. For initialisation from back-up, make sure that the back-up files are accessible from the system on which IUCLID will be initialised. What to do in each scenario is described in the rest of this chapter.

4.1. Starting IUCLID 5

Connect to the application by running the file named `iuclid5.cmd` that is supplied with the installation files. It is convenient to create a shortcut that points to `iuclid5.cmd` and to attach the IUCLID 5 icon that is supplied with the installation files.

Figure 4.1. A shortcut to the IUCLID 5 application

4.2. First steps wizard

When you start IUCLID 5 for the first time, the *First steps* wizard is run automatically. It guides you through the steps required to make a working user account and to upload the data required to use IUCLID 5 in a practical setting. The settings that relate to user accounts can also be changed after having run the wizard, using the features described in the IUCLID 5 User Manual.

Important

This wizard allows a single user account to be created, per run. This user is in addition to the *SuperUser* account that comes with the installation. It is essential to have at least one user account in addition to *SuperUser* because *SuperUser* should be used only for the special tasks that only it can carry out. See the IUCLID 5 User Manual for more detail.

As part of the First steps wizard, a legal entity must be uploaded into the IUCLID 5 installation in the form of a LEOX file. Therefore, before running this wizard, make sure that a LEOX file for the legal entity of your company or organisation is accessible to your computer. For more information, see the IUCLID 5 User Manual.

The First steps wizard provides the option of uploading the following information to your IUCLID 5 installation. For details, see the IUCLID 5 User Manual:

- EC Inventory
- Inventory of Reference substances

Although these uploads are optional, it is strongly recommended to do them during the first run of the First steps wizard. To do so, you will need to have the data accessible to your computer whilst running this wizard.

The First steps wizard can be run at any time, but only by the *SuperUser*. This is done from the file menu within IUCLID 5 **Administrative tools** / **Initialise**.

When starting the IUCLID 5 for the first time, the only user available is an administrator named *SuperUser*. Log in as *SuperUser* by entering the following case-sensitive values into the login screen as shown below:

Username: SuperUser

Password: root

The First steps wizard then proceeds. Each page of the wizard is described in a figure below.

Figure 4.2. Step 1 of the First steps wizard - Introduction

The wizard presents some useful information. There are no actions other than to read the information. Click the **Next** button.

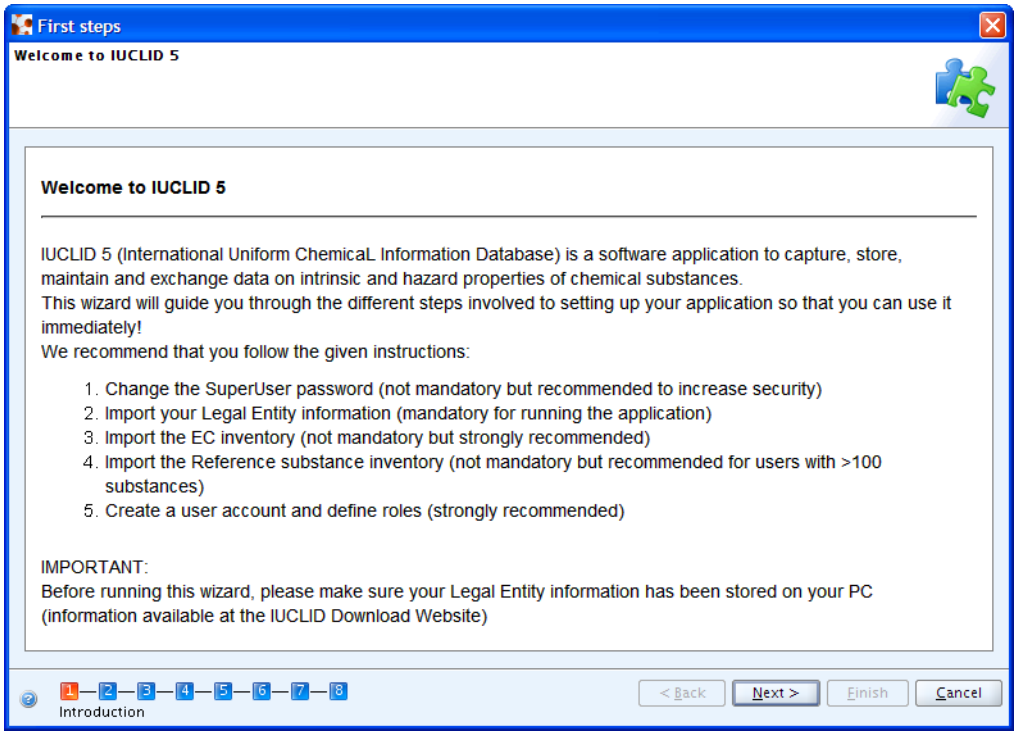

First steps
Welcome to IUCLID 5
Welcome to IUCLID 5
IUCLID 5 (International Uniform ChemicaL Information Database) is a software application to capture, store, maintain and exchange data on intrinsic and hazard properties of chemical substances.
This wizard will guide you through the different steps involved to setting up your application so that you can use it immediately!
We recommend that you follow the given instructions:
1. Change the SuperUser password (not mandatory but recommended to increase security)
2. Import your Legal Entity information (mandatory for running the application)
3. Import the EC inventory (not mandatory but strongly recommended)
4. Import the Reference substance inventory (not mandatory but recommended for users with >100 substances)
5. Create a user account and define roles (strongly recommended)
IMPORTANT:
Before running this wizard, please make sure your Legal Entity information has been stored on your PC (information available at the IUCLID Download Website)
1 2 3 4 5 6 7 8
Introduction
< Back
Next >
Finish
Cancel

Figure 4.3. Step 2 of the First steps wizard - Init mode - New installation

To initialise a new database, select the button `New Installation`as shown below and continue to the next step.

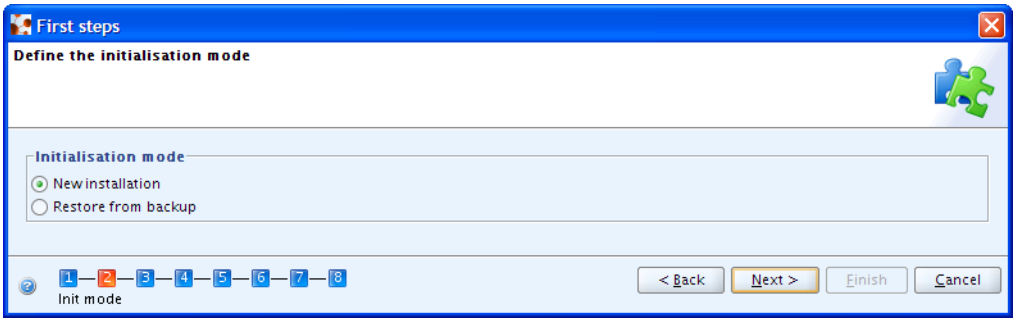
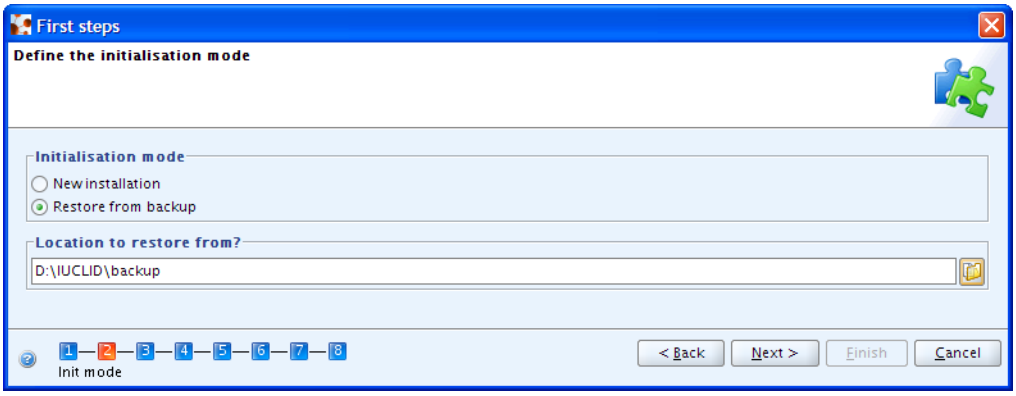


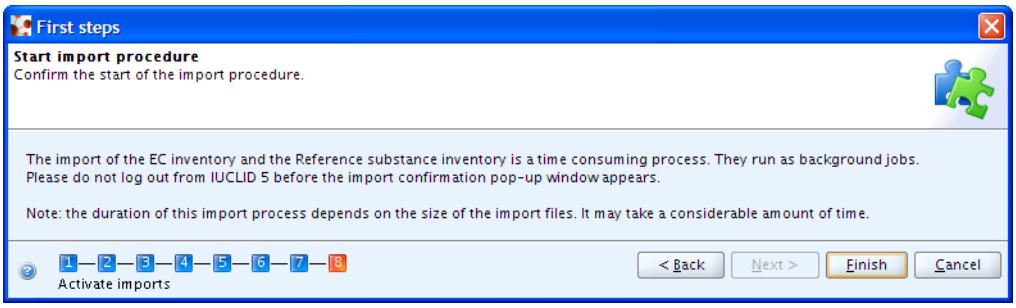
Figure 4.4. Step 2 of the First steps wizard - Init mode - Restore from backup

To restore from a backup of a previous version of IUCLID 5, select the button `Restore from backup` then enter the directory containing the backup files as shown in the example below.



Click **Next**. The wizard jumps to its last step, where the importation of data is started, as shown below.

Figure 4.5. Restoration from a back-up - Step 8 - Activate imports


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

The import may take some time. Click *Finish*. When the restoration is complete, the following screen is shown.

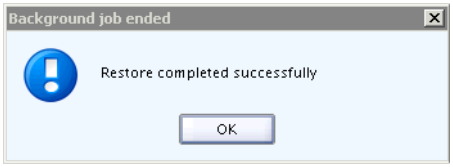


Figure 4.6. Step 3 of the First steps wizard - Change password

If you have not yet changed the default password of the *SuperUser* to a more secure value than *root*, the traffic light in the wizard screen will be yellow. To change the password, check the box `Change SuperUser password` , enter the old password *root* and then enter the new password. After confirming the password, click the button **Next**.

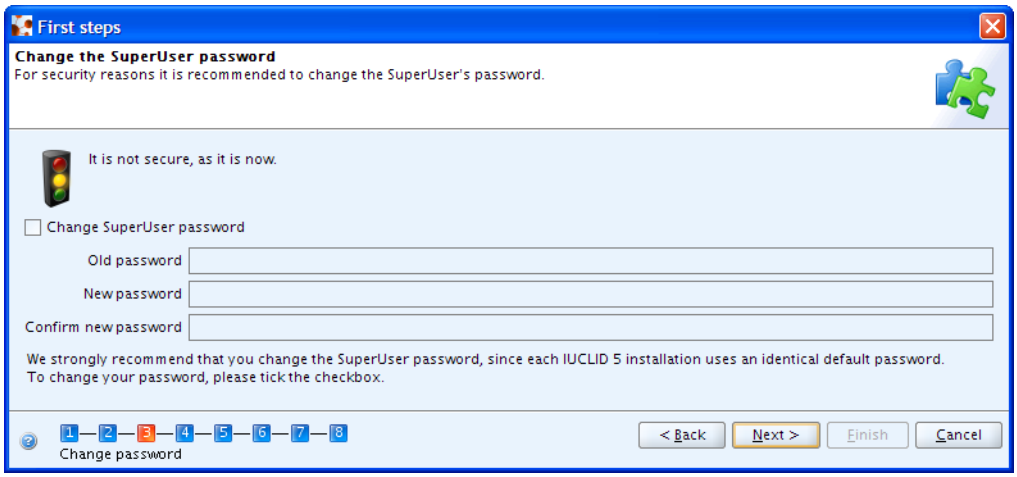
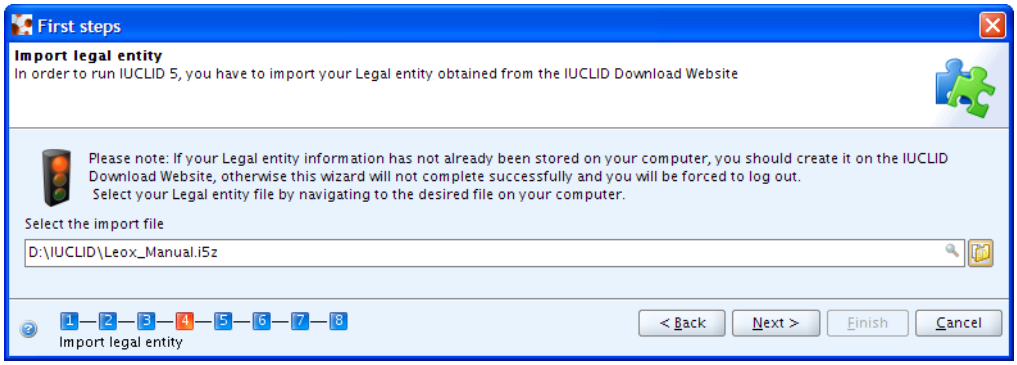
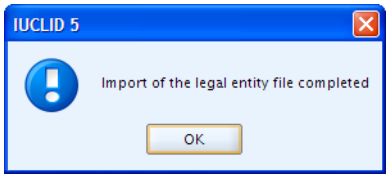

First steps
Change the SuperUser password
For security reasons it is recommended to change the SuperUser's password.
It is not secure, as it is now.
Change SuperUser password
Old password
New password
Confirm new password
We strongly recommend that you change the SuperUser password, since each IUCLID 5 installation uses an identical default password.
To change your password, please tick the checkbox.
1 2 3 4 5 6 7 8
Change password
< Back
Next >
Finish
Cancel

Figure 4.7. Step 4 of the First steps wizard - Import Legal Entity

To import a Legal entity (see the IUCLID 5 User Manual) select its LEOX file by browsing to the file. The browsing is accessed by clicking on the folder icon to the right of the field Select the import file. Click the **Next** button. The Legal entity is imported immediately.


First steps
Import legal entity
In order to run IUCLID 5, you have to import your Legal entity obtained from the IUCLID Download Website
Please note: If your Legal entity information has not already been stored on your computer, you should create it on the IUCLID Download Website, otherwise this wizard will not complete successfully and you will be forced to log out.
Select your Legal entity file by navigating to the desired file on your computer.
Select the import file
D:\IUCLID\Leox_Manual.i5z
1 2 3 4 5 6 7 8
Import legal entity
< Back
Next >
Finish
Cancel



Important

You must import at least one Legal entity in order to succeed with this wizard. If you have no Legal entity in the IUCLID 5 system, the traffic light in the wizard screen will be red. The First steps wizard will be automatically launched when you log in to IUCLID 5 until a Legal entity has been successfully imported.

Figure 4.8. Step 5 of the First steps wizard - Import EC Inventory

EC inventory import - To import the EC inventory, select the file for the EC inventory (see the IUCLID 5 User Manual). The EC Inventory will not be imported immediately. The import will start at the end of the First steps wizard. Depending on your machine speed and the size of the inventory, this import can take some time, e.g. up to half an hour.

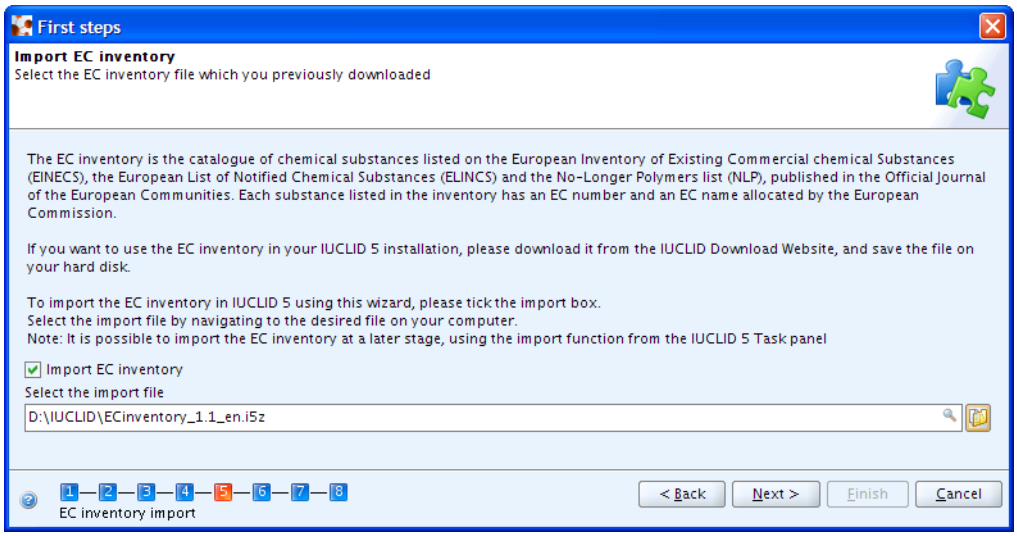
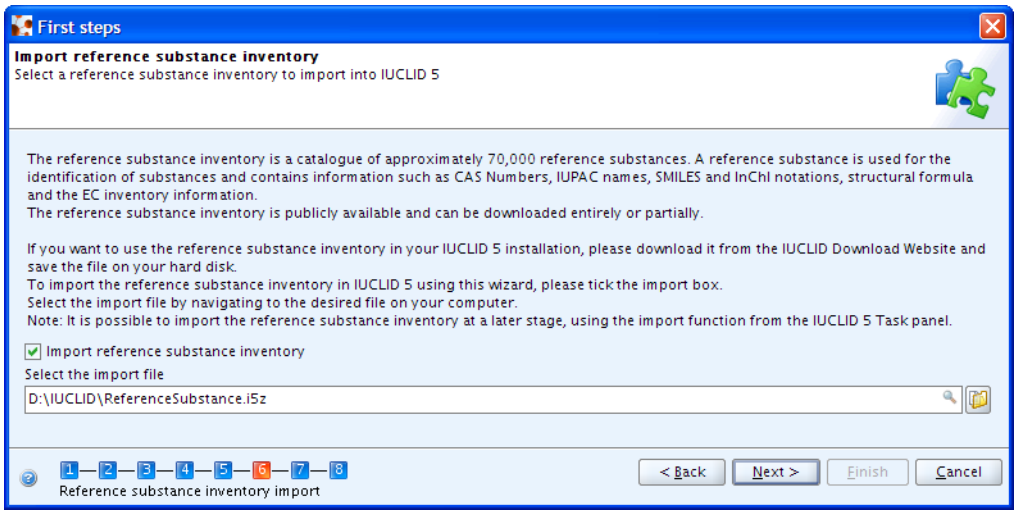

First steps
Import EC inventory
Select the EC inventory file which you previously downloaded
The EC inventory is the catalogue of chemical substances listed on the European Inventory of Existing Commercial chemical Substances (EINECS), the European List of Notified Chemical Substances (ELINCS) and the No-Longer Polymers list (NLP), published in the Official Journal of the European Communities. Each substance listed in the inventory has an EC number and an EC name allocated by the European Commission.
If you want to use the EC inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website, and save the file on your hard disk.
To import the EC inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the EC inventory at a later stage, using the import function from the IUCLID 5 Task panel
Import EC inventory
Select the import file
D:\IUCLID\ECinventory_1.1_en.i5z
1 2 3 4 5 6 7 8
EC inventory import
< Back
Next >
Finish
Cancel

Figure 4.9. Step 6 of the First steps wizard - Import reference substance inventory

Reference substance inventory import - Select the file for the Reference substance inventory (see the IUCLID 5 User Manual). The Reference substance inventory will not be imported immediately. The import will start at the end of the first steps wizard together with the EC Inventory import. Depending on your machine speed and the size of the inventory, this bulk operation may take a long time. The import of the Reference substance inventory itself can take **up to several hours**.

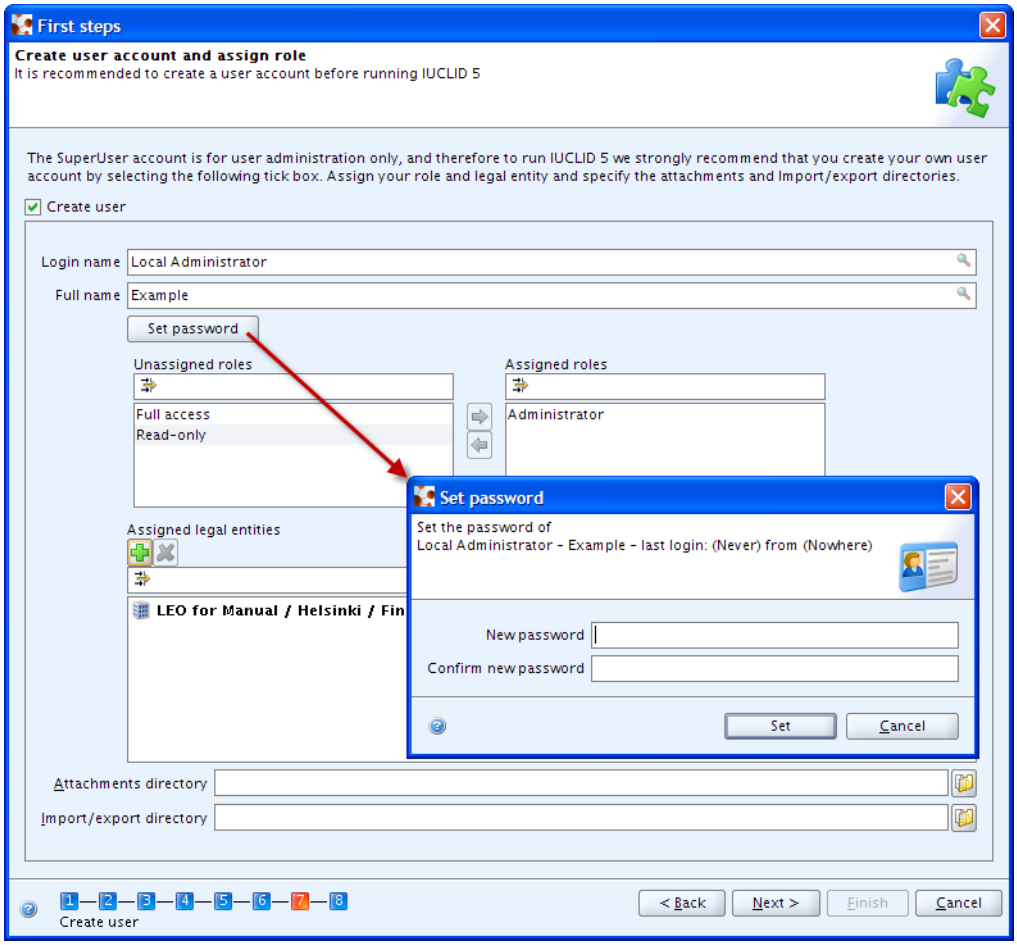

First steps
Import reference substance inventory
Select a reference substance inventory to import into IUCLID 5
The reference substance inventory is a catalogue of approximately 70,000 reference substances. A reference substance is used for the identification of substances and contains information such as CAS Numbers, IUPAC names, SMILES and InChI notations, structural formula and the EC inventory information.
The reference substance inventory is publicly available and can be downloaded entirely or partially.
If you want to use the reference substance inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website and save the file on your hard disk.
To import the reference substance inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the reference substance inventory at a later stage, using the import function from the IUCLID 5 Task panel.
Import reference substance inventory
Select the import file
D:\IUCLID\ReferenceSubstance.i5z
1 2 3 4 5 6 7 8
Reference substance inventory import
< Back
Next >
Finish
Cancel

Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set*, a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

Figure 4.10. Step 7 of the First steps wizard - Create user account and assign role

Create a new user account and define its user access rights by assigning it a role. It is essential to create a new user because general working within IUCLID 5 with the SuperUser is not supported. Only one user can be created per run of the First steps wizard.


First steps
Create user account and assign role
It is recommended to create a user account before running IUCLID 5
The SuperUser account is for user administration only, and therefore to run IUCLID 5 we strongly recommend that you create your own user account by selecting the following tick box. Assign your role and legal entity and specify the attachments and Import/export directories.
Create user
Login name
Local Administrator
Full name
Example
Set password
Unassigned roles
Full access
Read-only
Assigned roles
Administrator
Assigned legal entities
LEO for Manual / Helsinki / Fin
Set password
Set the password of
Local Administrator - Example - last login: (Never) from (Nowhere)
New password
Confirm new password
Set
Cancel
Attachments directory
Import/export directory
1 2 3 4 5 6 7 8
Create user
< Back
Next >
Finish
Cancel

- Select the checkbox `Create user`.

  Fill in all the fields. The user needs a `Login name` for identification during login. The `Full name` is used for proper user identification. The `Assigned role` is needed to administrate the access permissions. In a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default.

- Enter a `Login name`, as it should be used for identification during login, and the `Full name` used for proper user identification.

- Optionally, click Set password and define a password.

- Click and highlight a role in the list of unassigned roles and assign it to the user by clicking the Right arrow. Assigning a Role is needed to administrate the access permissions (in a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default).

Tip

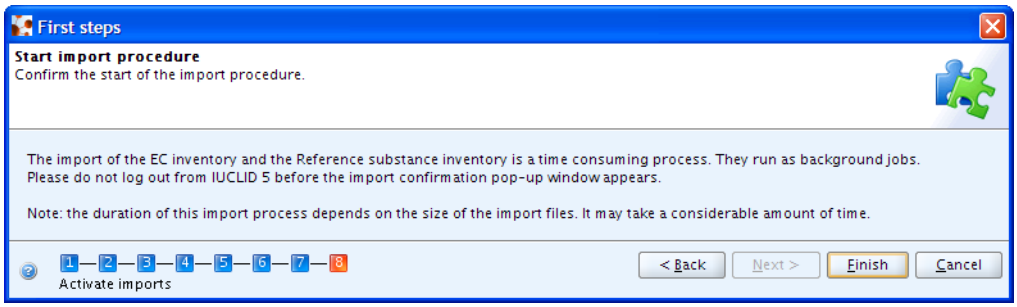
It is recommended to create a user with the *Administrator* Role regardless of whether a stand alone or a distributed version of IUCLID 5 is set up. Once a user has been created, the IUCLID 5 administrator (in case of a distributed version) can define different other user(s) and assign different role(s) to them (see the IUCLID 5 User Manual).

- Assign a Legal entity (normally the Legal entity imported in the third step of this wizard) by clicking the green plus button and performing a search for the desired Legal entity. In the Query field `Legal entity name`, enter the name of the desired Legal entity or an asterisk (*) as wildcard and click the **Search** button. In the Query results list, click the desired entry and then click the **Assign** button.
- Optionally, select default attachment and import/export directories. These settings can be changed at a later stage, as described in the IUCLID 5 User Manual.
- Click the **Next** button

Figure 4.11. Step 8 of the First steps wizard - Start import procedure

If you have selected an EC Inventory and/or Reference substances inventory file(s) during the wizard steps, you can now run the imports. Click the button **Execute imports**. Note again that these imports can take up to several hours, depending on your machine speed and the amount of data you are importing.

Then click the button **Finish**. If you have launched any imports, you will now have to wait until the imports are completed. Afterwards, you should log out and then log in again as a user for the newly defined account. Remember: general working as SuperUser is not supported.


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

4.3. User management

The installation of IUCLID 5 is now ready for hand-over to whoever will be maintaining the system and whoever will be managing the user accounts. The management of user accounts and their roles is described in the IUCLID 5 User Manual.

Chapter 5. Un-installation of IUCLID 5

The un-installation of IUCLID is a manual process. IUCLID can be un-installed by deleting the files that were copied to the destination machine, and reversing any changes made during the installation process. For more details about the actions that might be required, see the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.